Title: Quantum Spin Simulations (PHYS 7380) - Lecture 7

Date: Apr 13, 2010 11:00 AM

URL: http://pirsa.org/10040049

Abstract:

Pseudocode: using magnetization conservation

Constructing the basis in the block of $n_\uparrow$ spins ↑

Store state-integers in ordered list $\mathbf{s_a}$**, a=1,....,M**

```
do s = 0, 2^N - 1
    if (Σ_i s[i] = n↑) then a = a + 1; s_a = s endif
enddo
M = a
```

Example; N=4, $n_\uparrow$=2

$s_1=3$ (0011)

$s_2=5$ (0101)

$s_3=6$ (0110)

$s_4=9$ (1001)

$s_5=10$ (1010)

$s_6=12$ (1100)

How to locate a state (given integer s) in the list?

- stored map s→a would be too big for $s=0,\ldots,2^N-1$
- instead, we search the list s_a (here simplest way)

```
subroutine findstate(s, b)
b_min = 1; b_max = M
do
    b = b_min + (b_max - b_min)/2
    if (s < s_b) then
        b_max = b - 1
    elseif (s > s_b) then
        b_min = b + 1
    else
        exit
```

Finding the location ***b***
of a state-integer ***s*** in the list
- using bisection in the ordered list

Pseudocode: using magnetization conservation

Constructing the basis in the block of $n_\uparrow$ spins ↑

Store state-integers in ordered list s_a, $a=1,\ldots,M$

Example; $N=4$, $n_\uparrow=2$

do $s = 0, 2^N - 1$
  if $(\sum_i s[i] = n_\uparrow)$ **then** $a = a+1$; $s_a = s$ **endif**
enddo
$M = a$

$s_1=3$ (0011)
$s_2=5$ (0101)
$s_3=6$ (0110)
$s_4=9$ (1001)
$s_5=10$ (1010)
$s_6=12$ (1100)

How to locate a state (given integer s) in the list?

- stored map s→a would be too big for $s=0,\ldots,2^N-1$
- instead, we search the list s_a (here simplest way)

subroutine findstate(s, b)
$b_{\min} = 1$; $b_{\max} = M$
do
  $b = b_{\min} + (b_{\max} - b_{\min})/2$
  if $(s < s_b)$ **then**
    $b_{\max} = b - 1$
  elseif $(s > s_b)$ **then**
    $b_{\min} = b + 1$
  else
    exit

Finding the location ***b*** of a state-integer ***s*** in the list

- using bisection in the ordered list

Pseudocode; hamiltonian construction

- recall: states labeled a=1,...,M
- corresponding state-integers (bit representation) stored as s_a
- bit i, $s_a[i]$, corresponds to S^z_i

Pseudocode; hamiltonian construction

- recall: states labeled a=1,...,M
- corresponding state-integers (bit representation) stored as s_a
- bit i, $s_a[i]$, corresponds to S^z_i

```
do a = 1, M                                  loop over states
    do i = 0, N-1                            loop over sites
        j = mod(i+1, N)
        if (s_a[i] = s_a[j]) then            check bits of state-integers
            H(a,a) = H(a,a) + 1/4
        else
            H(a,a) = H(a,a) - 1/4
            s = flip(s_a, i, j)              state with bits i and j flipped
            call findstate(s, b)
            H(a,b) = H(a,b) + 1/2
        endif
    enddo
enddo
```

Momentum states (translationally invariant systems)

A periodic chain (ring), translationally invariant

- eigenstates with a fixed momentum (crystal momentum)
- quantum number k

$$T|n\rangle = e^{ik}|n\rangle \qquad k = m\frac{2\pi}{N}, \quad m = 0, \ldots, N-1,$$

Pseudocode: using magnetization conservation

Constructing the basis in the block of $n_\uparrow$ spins $\uparrow$

Store state-integers in ordered list **s_a, a=1,....,M**

$$
\begin{array}{l}
\textbf{do } s = 0, 2^N - 1 \\
\quad\quad \textbf{if } (\sum_i s[i] = n_\uparrow) \textbf{ then } a = a + 1;\ s_a = s \textbf{ endif} \\
\textbf{enddo} \\
M = a
\end{array}
$$

Pseudocode; hamiltonian construction

- recall: states labeled a=1,...,M
- corresponding state-integers (bit representation) stored as s_a
- bit i, $s_a[i]$, corresponds to S^z_i

Pseudocode; hamiltonian construction

- recall: states labeled a=1,...,M
- corresponding state-integers (bit representation) stored as s_a
- bit i, $s_a[i]$, corresponds to S^z_i

$$
\begin{array}{ll}
\textbf{do } a = 1, M & \text{loop over states} \\
\quad \textbf{do } i = 0, N-1 & \text{loop over sites} \\
\quad\quad j = \textbf{mod}(i+1, N) & \\
\quad\quad \textbf{if } (s_a[i] = s_a[j]) \textbf{ then} & \text{check bits of state-integers} \\
\quad\quad\quad H(a,a) = H(a,a) + \frac{1}{4} & \\
\quad\quad \textbf{else} & \\
\quad\quad\quad H(a,a) = H(a,a) - \frac{1}{4} & \\
\quad\quad\quad s = \textbf{flip}(s_a, i, j) & \text{state with bits i and j flipped} \\
\quad\quad\quad \textbf{call findstate}(s, b) & \\
\quad\quad\quad H(a,b) = H(a,b) + \frac{1}{2} & \\
\quad\quad \textbf{endif} & \\
\quad \textbf{enddo} & \\
\textbf{enddo} &
\end{array}
$$

Momentum states (translationally invariant systems)

A periodic chain (ring), translationally invariant

- eigenstates with a fixed momentum (crystal momentum)
- quantum number k

$$T|n\rangle = \mathrm{e}^{ik}|n\rangle \qquad k = m\frac{2\pi}{N}, \quad m = 0, \ldots, N-1,$$

The operator T translates the state by one lattice spacing

- for a spin basis state

$$T|S_1^z, S_2^z, \ldots, S_N^z\rangle = |S_N^z, S_1^z, \ldots, S_{N-1}^z\rangle$$

Momentum states (translationally invariant systems)

A periodic chain (ring), translationally invariant

- eigenstates with a fixed momentum (crystal momentum)
- quantum number k

$$T|n\rangle = \mathrm{e}^{ik}|n\rangle \qquad k = m\frac{2\pi}{N}, \quad m = 0, \ldots, N-1,$$

Momentum states (translationally invariant systems)

A periodic chain (ring), translationally invariant

- eigenstates with a fixed momentum (crystal momentum)
- quantum number k

$$T|n\rangle = \mathrm{e}^{ik}|n\rangle \qquad k = m\frac{2\pi}{N}, \quad m = 0, \ldots, N-1,$$

The operator T translates the state by one lattice spacing

- for a spin basis state

$$T|S_1^z, S_2^z, \ldots, S_N^z\rangle = |S_N^z, S_1^z, \ldots, S_{N-1}^z\rangle$$

Momentum states (translationally invariant systems)

A periodic chain (ring), translationally invariant

- eigenstates with a fixed momentum (crystal momentum)
- quantum number k

$$T|n\rangle = \mathrm{e}^{ik}|n\rangle \qquad k = m\frac{2\pi}{N}, \quad m = 0,\ldots,N-1,$$

The operator T translates the state by one lattice spacing

- for a spin basis state

$$T|S_1^z, S_2^z, \ldots, S_N^z\rangle = |S_N^z, S_1^z, \ldots, S_{N-1}^z\rangle$$

[T,H]=0 → momentum blocks of H

- can use eigenstates of T with given k as basis

Momentum states (translationally invariant systems)

A periodic chain (ring), translationally invariant

- eigenstates with a fixed momentum (crystal momentum)
- quantum number k

$$T|n\rangle = \mathrm{e}^{ik}|n\rangle \qquad k = m\frac{2\pi}{N}, \quad m = 0, \ldots, N-1,$$

The operator T translates the state by one lattice spacing

- for a spin basis state

$$T|S_1^z, S_2^z, \ldots, S_N^z\rangle = |S_N^z, S_1^z, \ldots, S_{N-1}^z\rangle$$

[T,H]=0 → momentum blocks of H

- can use eigenstates of T with given k as basis

also $[T,m_z]=0$ → m_z blocks split into momentum blocks of H

- construct basis for given (m_z,k)

Momentum states (translationally invariant systems)

A periodic chain (ring), translationally invariant

- eigenstates with a fixed momentum (crystal momentum)
- quantum number k

$$T|n\rangle = \mathrm{e}^{ik}|n\rangle \qquad k = m\frac{2\pi}{N}, \quad m = 0, \ldots, N-1,$$

The operator T translates the state by one lattice spacing

- for a spin basis state

$$T|S_1^z, S_2^z, \ldots, S_N^z\rangle = |S_N^z, S_1^z, \ldots, S_{N-1}^z\rangle$$

[T,H]=0 → momentum blocks of H

- can use eigenstates of T with given k as basis

also $[T,m_z]=0$ → m_z blocks split into momentum blocks of H

- construct basis for given (m_z,k)

We have to construct a complete basis of eigenstates of k or (m_z,k)

A momentum state can be constructed from a **representative** state la>

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle, \qquad |a\rangle = |S_1^z, \ldots, S_N^z\rangle$$

A momentum state can be constructed from a **representative** state |a>

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle, \qquad |a\rangle = |S_1^z, \ldots, S_N^z\rangle$$

Convention: A representative |a> must be a state with the the lowest binary-integer representation among all its translations

- If |a> and |b> are representatives, then

$$T^r|a\rangle \neq |b\rangle \quad r \in \{1, \ldots, N-1\}$$

|a> represents all its translations

4-site examples

(**0011**)→(0110),(1100),(1001)

(**0101**)→(1010)

A momentum state can be constructed from a **representative** state |a>

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle, \qquad |a\rangle = |S_1^z, \ldots, S_N^z\rangle$$

Convention: A representative |a> must be a state with the the lowest binary-integer representation among all its translations

- If |a> and |b> are representatives, then

$$T^r|a\rangle \neq |b\rangle \quad r \in \{1, \ldots, N-1\}$$

|a> represents all its translations

<u>4-site examples</u>

(**0011**)→(0110),(1100),(1001)

(**0101**)→(1010)

A momentum state can be constructed from a **representative** state la>

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} e^{-ikr} T^r |a\rangle, \qquad |a\rangle = |S_1^z, \ldots, S_N^z\rangle$$

Convention: A representative la> must be a state with the the lowest binary-integer representation among all its translations

- If la> and lb> are representatives, then

$$T^r|a\rangle \neq |b\rangle \quad r \in \{1, \ldots, N-1\}$$

la> represents all its translations

<u>4-site examples</u>

(**0011**)→(0110),(1100),(1001)

(**0101**)→(1010)

The sum can contain several copies of the same state (periodicity R):

$$T^R|a\rangle = |a\rangle \text{ for some } R$$

- the total weight for the component la> in la(k)> is

$$1 + e^{-ikR} + e^{-i2kR} + \ldots + e^{-ik(N/R-1)R}$$

- vanishes (state incompatible with k) unless kR=n2π
- the total weight of the representative is then N/R

A momentum state can be constructed from a **representative** state |a>

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle, \qquad |a\rangle = |S_1^z, \ldots, S_N^z\rangle$$

Convention: A representative |a> must be a state with the the lowest binary-integer representation among all its translations

- If |a> and |b> are representatives, then

$$T^r|a\rangle \neq |b\rangle \quad r \in \{1, \ldots, N-1\}$$

|a> represents all its translations

4-site examples

(**0011**)→(0110),(1100),(1001)

(**0101**)→(1010)

A momentum state can be constructed from a **representative** state |a>

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle, \qquad |a\rangle = |S_1^z, \ldots, S_N^z\rangle$$

Convention: A representative |a> must be a state with the the lowest binary-integer representation among all its translations

- If |a> and |b> are representatives, then

$$T^r|a\rangle \neq |b\rangle \quad r \in \{1, \ldots, N-1\}$$

|a> represents all its translations

<u>4-site examples</u>
(**0011**)→(0110),(1100),(1001)
(**0101**)→(1010)

The sum can contain several copies of the same state (periodicity R):

$$T^R|a\rangle = |a\rangle \ \text{ for some } R$$

- the total weight for the component |a> in |a(k)> is

$$1 + \mathrm{e}^{-ikR} + \mathrm{e}^{-i2kR} + \ldots + \mathrm{e}^{-ik(N/R-1)R}$$

- vanishes (state incompatible with k) unless kR=n2π
- the total weight of the representative is then N/R

A momentum state can be constructed from a **representative** state |a>

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle, \qquad |a\rangle = |S_1^z, \ldots, S_N^z\rangle$$

Convention: A representative |a> must be a state with the the lowest binary-integer representation among all its translations

- If |a> and |b> are representatives, then

$$T^r|a\rangle \neq |b\rangle \quad r \in \{1, \ldots, N-1\}$$

|a> represents all its translations

4-site examples
(**0011**)→(0110),(1100),(1001)
(**0101**)→(1010)

The sum can contain several copies of the same state (periodicity R):

$$T^R|a\rangle = |a\rangle \quad \text{for some } R$$

- the total weight for the component |a> in |a(k)> is

$$1 + \mathrm{e}^{-ikR} + \mathrm{e}^{-i2kR} + \ldots + \mathrm{e}^{-ik(N/R-1)R}$$

- vanishes (state incompatible with k) unless kR=n2π
- the total weight of the representative is then N/R

Condition for periodicity compatible with momentum k=m2π/N:

$$kR = n2\pi \rightarrow \frac{mR}{N} = n \rightarrow m = n\frac{N}{R} \rightarrow \mathrm{mod}(m, N/R) = 0$$

A momentum state can be constructed from a **representative** state |a>

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} e^{-ikr} T^r |a\rangle, \qquad |a\rangle = |S_1^z, \ldots, S_N^z\rangle$$

Convention: A representative |a> must be a state with the the lowest binary-integer representation among all its translations

- If |a> and |b> are representatives, then

$$T^r|a\rangle \neq |b\rangle \quad r \in \{1, \ldots, N-1\}$$

|a> represents all its translations

4-site examples
(**0011**)→(0110),(1100),(1001)
(**0101**)→(1010)

The sum can contain several copies of the same state (periodicity R):

$$T^R|a\rangle = |a\rangle \text{ for some } R$$

- the total weight for the component |a> in |a(k)> is

$$1 + e^{-ikR} + e^{-i2kR} + \ldots + e^{-ik(N/R-1)R}$$

- vanishes (state incompatible with k) unless kR=n2π
- the total weight of the representative is then N/R

Condition for periodicity compatible with momentum k=m2π/N:

$$kR = n2\pi \rightarrow \frac{mR}{N} = n \rightarrow m = n\frac{N}{R} \rightarrow \text{mod}(m, N/R) = 0$$

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle$$

Normalization of a state |*a*(k)> with periodicity R_a

$$\langle a(k)|a(k)\rangle = \frac{1}{N_a} \times R_a \times \left(\frac{N}{R_a}\right)^2 = 1 \rightarrow N_a = \frac{N^2}{R_a}$$

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle$$

Normalization of a state |*a*(k)> with periodicity R_a

$$\langle a(k)|a(k)\rangle = \frac{1}{N_a} \times R_a \times \left(\frac{N}{R_a}\right)^2 = 1 \rightarrow N_a = \frac{N^2}{R_a}$$

Pseudocode; basis construction

$\mathbf{do}\ s = 0, 2^N - 1$
  $\mathbf{call\ checkstate}(s, R)$
  $\mathbf{if}\ R \geq 0\ \mathbf{then}\ a = a + 1;\ s_a = s;\ R_a = R\ \mathbf{endif}$
$\mathbf{enddo}$
$M = a$

M = size of the H-block

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} e^{-ikr} T^r |a\rangle$$

Normalization of a state $|a(k)\rangle$ with periodicity R_a

$$\langle a(k)|a(k)\rangle = \frac{1}{N_a} \times R_a \times \left(\frac{N}{R_a}\right)^2 = 1 \rightarrow N_a = \frac{N^2}{R_a}$$

Pseudocode; basis construction

$$
\begin{aligned}
&\textbf{do } s = 0, 2^N - 1 \\
&\quad \textbf{call checkstate}(s, R) \\
&\quad \textbf{if } R \geq 0 \textbf{ then } a = a + 1;\ s_a = s;\ R_a = R \textbf{ endif} \\
&\textbf{enddo} \\
&M = a
\end{aligned}
$$

M = size of the H-block

Uses a subroutine **checkstate**(s,R)

- R = periodicity if state-integer s is a new representative
- store in list ***R_a*, *a*=1,...,*M***
- $R = -1$ if
  - the magnetization is not the one currently considered

Translations of the representative; cyclic permutation

Define function **cyclebits**(t,N)

- cyclic permutations of first N bits of integer t
- F90 function ishiftc(t,−1,N)

Translations of the representative; cyclic permutation

Define function **cyclebits**(t,N)

- cyclic permutations of first N bits of integer t
- F90 function ishiftc(t,–1,N)

The representative has the lowest state-integer among all its translations

Translations of the representative; cyclic permutation

Define function **cyclebits**(t,N)

- cyclic permutations of first N bits of integer t
- F90 function ishiftc(t,–1,N)

The representative has the lowest state-integer among all its translations

Pseudocode; checkstate() subroutine

subroutine checkstate(s, R)
$R = -1$
if $(\sum_i s[i] \neq n_\uparrow)$ **return**
$t = s$
do $i = 1, N$
    $t =$ **cyclebits**(t, N)
    if $(t < s)$ **then**
        return
    elseif $(t = s)$ **then**
        if (**mod**$(k, N/i) \neq 0$) **return**
        $R = i$; **return**
    endif

check the magnetization

check if translated state has lower integer representation

check momentum compatibility

- k is the integer corresponding to the momentum; k=0,...,N-1

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle$$

Normalization of a state |*a*(k)> with periodicity R_a

$$\langle a(k)|a(k)\rangle = \frac{1}{N_a} \times R_a \times \left(\frac{N}{R_a}\right)^2 = 1 \rightarrow N_a = \frac{N^2}{R_a}$$

A momentum state can be constructed from a **representative** state la>

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle, \qquad |a\rangle = |S_1^z, \ldots, S_N^z\rangle$$

A momentum state can be constructed from a **representative** state la>

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle, \qquad |a\rangle = |S_1^z, \ldots, S_N^z\rangle$$

Convention: A representative la> must be a state with the the lowest binary-integer representation among all its translations

- If la> and lb> are representatives, then

$$T^r|a\rangle \neq |b\rangle \quad r \in \{1, \ldots, N-1\}$$

la> represents all its translations

4-site examples

(**0011**)→(0110),(1100),(1001)

(**0101**)→(1010)

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle$$

Normalization of a state |*a*(k)> with periodicity R_a

$$\langle a(k)|a(k)\rangle = \frac{1}{N_a} \times R_a \times \left(\frac{N}{R_a}\right)^2 = 1 \rightarrow N_a = \frac{N^2}{R_a}$$

Translations of the representative; cyclic permutation

Define function **cyclebits**(t,N)

- cyclic permutations of first N bits of integer t
- F90 function ishiftc(t,−1,N)

Translations of the representative; cyclic permutation

Define function **cyclebits**(t,N)

- cyclic permutations of first N bits of integer t
- F90 function ishiftc(t,–1,N)

The representative has the lowest state-integer among all its translations

Pseudocode; checkstate() subroutine

subroutine checkstate(s, R)
$R = -1$
if $(\sum_i s[i] \neq n_\uparrow)$ **return**
$t = s$
do $i = 1, N$
    $t =$ **cyclebits**(t, N)
    if $(t < s)$ **then**
        return
    elseif $(t = s)$ **then**
        if $(\mathbf{mod}(k, N/i) \neq 0)$ **return**
        $R = i$; **return**
    endif

check the magnetization

check if translated state has lower integer representation

check momentum compatibility

- k is the integer corresponding to the momentum; k=0,...,N-1

The Hamiltonian matrix. Write $S = 1/2$ chain hamiltonian as

$$H_0 = \sum_{j=1}^{N} S_j^z S_{j+1}^z, \quad H_j = \frac{1}{2}(S_j^+ S_{j+1}^- + S_j^+ S_{j+1}^-), \quad j = 1, \ldots, N$$

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle$$

Normalization of a state $|a(k)\rangle$ with periodicity R_a

$$\langle a(k)|a(k)\rangle = \frac{1}{N_a} \times R_a \times \left(\frac{N}{R_a}\right)^2 = 1 \rightarrow N_a = \frac{N^2}{R_a}$$

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle$$

Normalization of a state |*a*(k)> with periodicity R_a

$$\langle a(k)|a(k)\rangle = \frac{1}{N_a} \times R_a \times \left(\frac{N}{R_a}\right)^2 = 1 \rightarrow N_a = \frac{N^2}{R_a}$$

Pseudocode; basis construction

$\mathbf{do}\ s = 0, 2^N - 1$
$\quad \mathbf{call\ checkstate}(s, R)$
$\quad \mathbf{if}\ R \geq 0\ \mathbf{then}\ a = a + 1;\ s_a = s;\ R_a = R\ \mathbf{endif}$
$\mathbf{enddo}$
$M = a$

M = size of the H-block

Translations of the representative; cyclic permutation

Define function **cyclebits**(t,N)

- cyclic permutations of first N bits of integer t
- F90 function ishiftc(t,–1,N)

The representative has the lowest state-integer among all its translations

Pseudocode; checkstate() subroutine

```
subroutine checkstate(s, R)
R = −1
if (∑_i s[i] ≠ n↑) return
t = s
do i = 1, N
     t = cyclebits(t, N)
     if (t < s) then
          return
     elseif (t = s) then
          if (mod(k, N/i) ≠ 0) return
          R = i; return
     endif
```

check the magnetization

check if translated state has lower integer representation

check momentum compatibility

- k is the integer corresponding to the momentum; k=0,...,N-1

The Hamiltonian matrix. Write $S = 1/2$ chain hamiltonian as

$$H_0 = \sum_{j=1}^{N} S_j^z S_{j+1}^z, \quad H_j = \frac{1}{2}(S_j^+ S_{j+1}^- + S_j^+ S_{j+1}^-), \quad j = 1, \ldots, N$$

The Hamiltonian matrix. Write $S = 1/2$ chain hamiltonian as

$$H_0 = \sum_{j=1}^{N} S^z_j S^z_{j+1}, \quad H_j = \tfrac{1}{2}(S^+_j S^-_{j+1} + S^+_j S^-_{j+1}), \quad j = 1, \ldots, N$$

Act with H on a momentum state; use [H,T]=0

$$H|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r H|a\rangle = \frac{1}{\sqrt{N_a}} \sum_{j=0}^{N} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r H_j|a\rangle,$$

The Hamiltonian matrix. Write $S = 1/2$ chain hamiltonian as

$$H_0 = \sum_{j=1}^{N} S^z_j S^z_{j+1}, \quad H_j = \tfrac{1}{2}(S^+_j S^-_{j+1} + S^+_j S^-_{j+1}), \quad j = 1, \ldots, N$$

Act with H on a momentum state; use [H,T]=0

$$H|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r H|a\rangle = \frac{1}{\sqrt{N_a}} \sum_{j=0}^{N} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r H_j |a\rangle,$$

$H_j|a\rangle$ is related to some representative: $H_j|a\rangle = h^j_a T^{-l_j} |b_j\rangle$

$$H|a(k)\rangle = \sum_{j=0}^{N} \frac{h^j_a}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^{(r-l_j)} |b_j\rangle$$

The Hamiltonian matrix. Write $S = 1/2$ chain hamiltonian as

$$H_0 = \sum_{j=1}^{N} S_j^z S_{j+1}^z, \quad H_j = \tfrac{1}{2}(S_j^+ S_{j+1}^- + S_j^+ S_{j+1}^-), \;\; j = 1, \ldots, N$$

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle$$

Normalization of a state |*a*(k)> with periodicity R_a

$$\langle a(k)|a(k)\rangle = \frac{1}{N_a} \times R_a \times \left(\frac{N}{R_a}\right)^2 = 1 \rightarrow N_a = \frac{N^2}{R_a}$$

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle$$

Normalization of a state |*a*(k)> with periodicity R_a

$$\langle a(k)|a(k)\rangle = \frac{1}{N_a} \times R_a \times \left(\frac{N}{R_a}\right)^2 = 1 \rightarrow N_a = \frac{N^2}{R_a}$$

A momentum state can be constructed from a **representative** state |a>

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle, \quad |a\rangle = |S_1^z, \ldots, S_N^z\rangle$$

Convention: A representative |a> must be a state with the the lowest binary-integer representation among all its translations

- If |a> and |b> are representatives, then

$$T^r |a\rangle \neq |b\rangle \quad r \in \{1, \ldots, N-1\}$$

|a> represents all its translations

4-site examples

(**0011**)→(0110),(1100),(1001)

(**0101**)→(1010)

Translations of the representative; cyclic permutation

Define function **cyclebits**(t,N)

- cyclic permutations of first N bits of integer t
- F90 function ishiftc(t,−1,N)

Translations of the representative; cyclic permutation

Define function **cyclebits**(t,N)

- cyclic permutations of first N bits of integer t
- F90 function ishiftc(t,–1,N)

The representative has the lowest state-integer among all its translations

Pseudocode; checkstate() subroutine

subroutine checkstate(s, R)
$R = -1$
if $(\sum_i s[i] \neq n_\uparrow)$ **return**
$t = s$
do $i = 1, N$
    $t =$ **cyclebits**(t, N)
    if $(t < s)$ **then**
        return
    elseif $(t = s)$ **then**
        if $($**mod**$(k, N/i) \neq 0)$ **return**
        $R = i$; **return**
    endif

check the magnetization

check if translated state has lower integer representation

check momentum compatibility

- k is the integer corresponding to the momentum; k=0,...,N-1

The Hamiltonian matrix. Write $S = 1/2$ chain hamiltonian as

$$H_0 = \sum_{j=1}^{N} S^z_j S^z_{j+1}, \quad H_j = \tfrac{1}{2}(S^+_j S^-_{j+1} + S^+_j S^-_{j+1}), \quad j = 1, \ldots, N$$

Act with H on a momentum state; use [H,T]=0

$$H|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r H|a\rangle = \frac{1}{\sqrt{N_a}} \sum_{j=0}^{N} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r H_j|a\rangle,$$

$H_j|a\rangle$ is related to some representative: $H_j|a\rangle = h^j_a T^{-l_j}|b_j\rangle$

$$H|a(k)\rangle = \sum_{j=0}^{N} \frac{h^j_a}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^{(r-l_j)}|b_j\rangle$$

The Hamiltonian matrix. Write $S = 1/2$ chain hamiltonian as

$$H_0 = \sum_{j=1}^{N} S^z_j S^z_{j+1}, \quad H_j = \tfrac{1}{2}(S^+_j S^-_{j+1} + S^+_j S^-_{j+1}), \quad j = 1, \ldots, N$$

Act with H on a momentum state; use [H,T]=0

$$H|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r H|a\rangle = \frac{1}{\sqrt{N_a}} \sum_{j=0}^{N} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r H_j|a\rangle,$$

$H_j|a\rangle$ is related to some representative: $H_j|a\rangle = h^j_a T^{-l_j}|b_j\rangle$

$$H|a(k)\rangle = \sum_{j=0}^{N} \frac{h^j_a}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^{(r-l_j)}|b_j\rangle$$

Shift summation index r and use definition of momentum state

$$H|a(k)\rangle = \sum_{j=0}^{N} h^j_a \mathrm{e}^{-ikl_j} \sqrt{\frac{N_{b_j}}{N_a}} |b_j(k)\rangle$$ → matrix elements

$$\langle a(k)|H_0|a(k)\rangle = \sum_{j=1}^{N} S^z_j S^z_j,$$

Pseudocode; hamiltonian construction

First, some elements needed; recall

$$H_j|a\rangle = h_a^j T^{-l_j}|b_j\rangle$$

Pseudocode; hamiltonian construction

First, some elements needed; recall

$$H_j|a\rangle = h_a^j T^{-l_j}|b_j\rangle$$

Finding the representative r of a state-integer s

- lowest integer among all translations

$$|r\rangle = T^l|s\rangle$$

```
subroutine representative(s, r, l)
r = s; t = s; l = 0
do i = 1, N - 1
     t = cyclebits(t, N)
     if (t < r) then r = t; l = i endif
enddo
```

Pseudocode; hamiltonian construction

First, some elements needed; recall

$$H_j|a\rangle = h_a^j T^{-l_j}|b_j\rangle$$

Finding the representative r of a state-integer s

- lowest integer among all translations

```
subroutine representative(s, r, l)
r = s; t = s; l = 0
do i = 1, N − 1
    t = cyclebits(t, N)
    if (t < r) then r = t; l = i endif
enddo
```

$$|r\rangle = T^l|s\rangle$$

```
subroutine findstate(s, b)
b_min = 1; b_max = M
do
    b = b_min + (b_max − b_min)/2
    if (s < s_b) then
        b_max = b − 1
    elseif (s > s_b) then
        b_min = b + 1
    else
        exit
    endif
    if (b_min > b_max then
        b = −1; exit
```

Finding the location of the representative in the state list

- may not be there, if the new state is incompatible with k
- **b=–1** for not found in list

Pseudocode; hamiltonian construction

First, some elements needed; recall

$$H_j|a\rangle = h_a^j T^{-l_j}|b_j\rangle$$

Pseudocode; hamiltonian construction

First, some elements needed; recall

$$H_j|a\rangle = h_a^j T^{-l_j}|b_j\rangle$$

Finding the representative r of a state-integer s
- lowest integer among all translations

$$
\begin{array}{l}
\textbf{subroutine representative}(s,r,l)\\
r=s;\ t=s;\ l=0\\
\textbf{do}\ i=1,N-1\\
\quad t=\textbf{cyclebits}(t,N)\\
\quad \textbf{if}\ (t<r)\ \textbf{then}\ r=t;\ l=i\ \textbf{endif}\\
\textbf{enddo}
\end{array}
$$

$$|r\rangle = T^l|s\rangle$$

Finding the location of the representative in the state list
- may not be there, if the new state is incompatible with k
- **b=–1** for not found in list

$$
\begin{array}{l}
\textbf{subroutine findstate}(s,b)\\
b_{\min}=1;\ b_{\max}=M\\
\textbf{do}\\
\quad b=b_{\min}+(b_{\max}-b_{\min})/2\\
\quad \textbf{if}\ (s<s_b)\ \textbf{then}\\
\qquad b_{\max}=b-1\\
\quad \textbf{elseif}\ (s>s_b)\ \textbf{then}\\
\qquad b_{\min}=b+1\\
\quad \textbf{else}\\
\qquad \textbf{exit}\\
\quad \textbf{endif}\\
\quad \textbf{if}\ (b_{\min}>b_{\max}\ \textbf{then}\\
\qquad b=-1;\ \textbf{exit}
\end{array}
$$

Construct all the matrix elements

do $a = 1, M$
  do $i = 0, N-1$
    $j = \mathbf{mod}(i+1, N)$
    if $(s_a[i] = s_a[j])$ **then**
      $H(a,a) = H(a,a) + \frac{1}{4}$
    else
      $H(a,a) = H(a,a) - \frac{1}{4}$
      $s = \mathbf{flip}(s_a, i, j)$
      call representative(s, r, l)
      call findstate(r, b)
      if $(b \geq 0)$ **then**
        $H(a,b) = H(a,b) + \frac{1}{2}\sqrt{R_a/R_b}\mathrm{e}^{i2\pi kl/N}$
      endif
    endif
  enddo
enddo

Construct all the matrix elements

$$
\begin{array}{l}
\textbf{do } a = 1, M \\
\quad \textbf{do } i = 0, N-1 \\
\quad\quad j = \textbf{mod}(i+1, N) \\
\quad\quad \textbf{if } (s_a[i] = s_a[j]) \textbf{ then} \\
\quad\quad\quad H(a,a) = H(a,a) + \frac{1}{4} \\
\quad\quad \textbf{else} \\
\quad\quad\quad H(a,a) = H(a,a) - \frac{1}{4} \\
\quad\quad\quad s = \textbf{flip}(s_a, i, j) \\
\quad\quad\quad \textbf{call representative}(s, r, l) \\
\quad\quad\quad \textbf{call findstate}(r, b) \\
\quad\quad\quad \textbf{if } (b \geq 0) \textbf{ then} \\
\quad\quad\quad\quad H(a,b) = H(a,b) + \frac{1}{2}\sqrt{R_a/R_b}\,\mathrm{e}^{i2\pi kl/N} \\
\quad\quad\quad \textbf{endif} \\
\quad\quad \textbf{endif} \\
\quad \textbf{enddo} \\
\textbf{enddo}
\end{array}
$$

Pseudocode; hamiltonian construction

First, some elements needed; recall

$$H_j|a\rangle = h_a^j T^{-l_j}|b_j\rangle$$

Finding the representative r of a state-integer s

- lowest integer among all translations

$$|r\rangle = T^l|s\rangle$$

```
subroutine representative(s, r, l)
r = s; t = s; l = 0
do i = 1, N − 1
    t = cyclebits(t, N)
    if (t < r) then r = t; l = i endif
enddo
```

Finding the location of the representative in the state list

- may not be there, if the new state is incompatible with k
- **b=–1** for not found in list

```
subroutine findstate(s, b)
b_min = 1; b_max = M
do
    b = b_min + (b_max − b_min)/2
    if (s < s_b) then
        b_max = b − 1
    elseif (s > s_b) then
        b_min = b + 1
    else
        exit
    endif
    if (b_min > b_max then
        b = −1; exit
```

Pseudocode; hamiltonian construction

First, some elements needed; recall

$$H_j|a\rangle = h_a^j T^{-l_j}|b_j\rangle$$

The Hamiltonian matrix. Write $S = 1/2$ chain hamiltonian as

$$H_0 = \sum_{j=1}^{N} S_j^z S_{j+1}^z, \quad H_j = \tfrac{1}{2}(S_j^+ S_{j+1}^- + S_j^+ S_{j+1}^-), \quad j = 1, \ldots, N$$

The Hamiltonian matrix. Write $S = 1/2$ chain hamiltonian as

$$H_0 = \sum_{j=1}^{N} S^z_j S^z_{j+1}, \quad H_j = \tfrac{1}{2}(S^+_j S^-_{j+1} + S^+_j S^-_{j+1}), \;\; j = 1, \ldots, N$$

Act with H on a momentum state; use [H,T]=0

$$H|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r H|a\rangle = \frac{1}{\sqrt{N_a}} \sum_{j=0}^{N} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r H_j|a\rangle,$$

$H_j|a\rangle$ is related to some representative: $H_j|a\rangle = h^j_a T^{-l_j}|b_j\rangle$

$$H|a(k)\rangle = \sum_{j=0}^{N} \frac{h^j_a}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^{(r-l_j)}|b_j\rangle$$

Shift summation index r and use definition of momentum state

$$H|a(k)\rangle = \sum_{j=0}^{N} h^j_a \mathrm{e}^{-ikl_j} \sqrt{\frac{N_{b_j}}{N_a}}|b_j(k)\rangle$$ → matrix elements

$$\langle a(k)|H_0|a(k)\rangle = \sum_{j=1}^{N} S^z_j S^z_j,$$

A momentum state can be constructed from a **representative** state la>

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle, \qquad |a\rangle = |S_1^z, \ldots, S_N^z\rangle$$

A momentum state can be constructed from a **representative** state |a>

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} e^{-ikr} T^r |a\rangle, \quad |a\rangle = |S_1^z, \ldots, S_N^z\rangle$$

Convention: A representative |a> must be a state with the the lowest binary-integer representation among all its translations

- If |a> and |b> are representatives, then

$$T^r|a\rangle \neq |b\rangle \quad r \in \{1, \ldots, N-1\}$$

|a> represents all its translations

4-site examples
(**0011**)→(0110),(1100),(1001)
(**0101**)→(1010)

The sum can contain several copies of the same state (periodicity R):

$$T^R|a\rangle = |a\rangle \quad \text{for some } R$$

- the total weight for the component |a> in |a(k)> is

$$1 + e^{-ikR} + e^{-i2kR} + \ldots + e^{-ik(N/R-1)R}$$

- vanishes (state incompatible with k) unless kR=n2π
- the total weight of the representative is then N/R

Condition for periodicity compatible with momentum k=m2π/N:

$$kR = n2\pi \rightarrow \frac{mR}{N} = n \rightarrow m = n\frac{N}{R} \rightarrow \text{mod}(m, N/R) = 0$$

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} e^{-ikr} T^r |a\rangle$$

Normalization of a state |*a*(k)> with periodicity R_a

$$\langle a(k)|a(k)\rangle = \frac{1}{N_a} \times R_a \times \left(\frac{N}{R_a}\right)^2 = 1 \rightarrow N_a = \frac{N^2}{R_a}$$

Pseudocode; basis construction

do $s = 0, 2^N - 1$
    call checkstate(s, R)
    if $R \geq 0$ **then** $a = a + 1;\ s_a = s;\ R_a = R$ **endif**
enddo
$M = a$

M = size of the H-block

Uses a subroutine **checkstate**(s,R)

- *R* = periodicity if state-integer s is a new representative
- store in list ***R_a*, *a*=1,...,*M***
- *R* = −1 if
  - the magnetization is not the one currently considered

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle$$

Normalization of a state $|a(k)\rangle$ with periodicity R_a

$$\langle a(k)|a(k)\rangle = \frac{1}{N_a} \times R_a \times \left(\frac{N}{R_a}\right)^2 = 1 \to N_a = \frac{N^2}{R_a}$$

Pseudocode; basis construction

```
do s = 0, 2^N − 1
    call checkstate(s, R)
    if R ≥ 0 then a = a + 1; s_a = s; R_a = R endif
enddo
M = a
```

M = size of the H-block

Uses a subroutine **checkstate**(s,R)

- R = periodicity if state-integer s is a new representative
- store in list ***R_a, a=1,...,M***
- $R = -1$ if
  - the magnetization is not the one currently considered

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle$$

Normalization of a state |*a*(k)> with periodicity R_a

$$\langle a(k)|a(k)\rangle = \frac{1}{N_a} \times R_a \times \left(\frac{N}{R_a}\right)^2 = 1 \rightarrow N_a = \frac{N^2}{R_a}$$

A momentum state can be constructed from a **representative** state |a>

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle, \qquad |a\rangle = |S_1^z, \ldots, S_N^z\rangle$$

Convention: A representative |a> must be a state with the the lowest binary-integer representation among all its translations

- If |a> and |b> are representatives, then

$$T^r|a\rangle \neq |b\rangle \quad r \in \{1, \ldots, N-1\}$$

|a> represents all its translations

4-site examples
(**0011**)→(0110),(1100),(1001)
(**0101**)→(1010)

The sum can contain several copies of the same state (periodicity R):

$$T^R|a\rangle = |a\rangle \text{ for some } R$$

- the total weight for the component |a> in |a(k)> is

$$1 + \mathrm{e}^{-ikR} + \mathrm{e}^{-i2kR} + \ldots + \mathrm{e}^{-ik(N/R-1)R}$$

- vanishes (state incompatible with k) unless kR=n2π
- the total weight of the representative is then N/R

Condition for periodicity compatible with momentum k=m2π/N:

$$kR = n2\pi \rightarrow \frac{mR}{N} = n \rightarrow m = n\frac{N}{R} \rightarrow \mathrm{mod}(m, N/R) = 0$$

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} e^{-ikr} T^r |a\rangle$$

Normalization of a state |*a*(k)> with periodicity R_a

$$\langle a(k)|a(k)\rangle = \frac{1}{N_a} \times R_a \times \left(\frac{N}{R_a}\right)^2 = 1 \rightarrow N_a = \frac{N^2}{R_a}$$

Pseudocode; basis construction

$$
\begin{array}{l}
\textbf{do } s = 0, 2^N - 1 \\
\quad \textbf{call checkstate}(s, R) \\
\quad \textbf{if } R \geq 0 \textbf{ then } a = a + 1;\ s_a = s;\ R_a = R \textbf{ endif} \\
\textbf{enddo} \\
M = a
\end{array}
$$

M = size of the H-block

Uses a subroutine **checkstate**(s,R)

- *R* = periodicity if state-integer s is a new representative
- store in list ***R*a, *a*=1,...,*M***
- *R* = −1 if
  - the magnetization is not the one currently considered

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle$$

Normalization of a state |*a*(k)> with periodicity R_a

$$\langle a(k)|a(k)\rangle = \frac{1}{N_a} \times R_a \times \left(\frac{N}{R_a}\right)^2 = 1 \rightarrow N_a = \frac{N^2}{R_a}$$

A momentum state can be constructed from a **representative** state |a>

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle, \qquad |a\rangle = |S_1^z, \ldots, S_N^z\rangle$$

Convention: A representative |a> must be a state with the the lowest binary-integer representation among all its translations

- If |a> and |b> are representatives, then

$$T^r|a\rangle \neq |b\rangle \quad r \in \{1, \ldots, N-1\}$$

|a> represents all its translations

4-site examples

(**0011**)→(0110),(1100),(1001)

(**0101**)→(1010)

Momentum states (translationally invariant systems)

A periodic chain (ring), translationally invariant

- eigenstates with a fixed momentum (crystal momentum)
- quantum number k

$$T|n\rangle = \mathrm{e}^{ik}|n\rangle \qquad k = m\frac{2\pi}{N}, \quad m = 0,\ldots,N-1,$$

The operator T translates the state by one lattice spacing

- for a spin basis state

$$T|S_1^z, S_2^z, \ldots, S_N^z\rangle = |S_N^z, S_1^z, \ldots, S_{N-1}^z\rangle$$

A momentum state can be constructed from a **representative** state |a>

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle, \qquad |a\rangle = |S_1^z, \ldots, S_N^z\rangle$$

Convention: A representative |a> must be a state with the the lowest binary-integer representation among all its translations

- If |a> and |b> are representatives, then

$$T^r|a\rangle \neq |b\rangle \quad r \in \{1, \ldots, N-1\}$$

|a> represents all its translations

4-site examples

(**0011**)→(0110),(1100),(1001)

(**0101**)→(1010)

The sum can contain several copies of the same state (periodicity R):

$$T^R|a\rangle = |a\rangle \ \text{ for some } R$$

- the total weight for the component |a> in |a(k)> is

$$1 + \mathrm{e}^{-ikR} + \mathrm{e}^{-i2kR} + \ldots + \mathrm{e}^{-ik(N/R-1)R}$$

- vanishes (state incompatible with k) unless kR=n2π
- the total weight of the representative is then N/R

A momentum state can be constructed from a **representative** state |a>

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle, \qquad |a\rangle = |S_1^z, \ldots, S_N^z\rangle$$

Convention: A representative |a> must be a state with the the lowest binary-integer representation among all its translations

- If |a> and |b> are representatives, then

$$T^r|a\rangle \neq |b\rangle \quad r \in \{1, \ldots, N-1\}$$

|a> represents all its translations

<u>4-site examples</u>
(**0011**)→(0110),(1100),(1001)
(**0101**)→(1010)

The sum can contain several copies of the same state (periodicity R):

$$T^R|a\rangle = |a\rangle \quad \text{for some } R$$

- the total weight for the component |a> in |a(k)> is

$$1 + \mathrm{e}^{-ikR} + \mathrm{e}^{-i2kR} + \ldots + \mathrm{e}^{-ik(N/R-1)R}$$

- vanishes (state incompatible with k) unless kR=n2π
- the total weight of the representative is then N/R

Condition for periodicity compatible with momentum k=m2π/N:

$$kR = n2\pi \rightarrow \frac{mR}{N} = n \rightarrow m = n\frac{N}{R} \rightarrow \mathrm{mod}(m, N/R) = 0$$

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle$$

Normalization of a state $|a(k)\rangle$ with periodicity R_a

$$\langle a(k)|a(k)\rangle = \frac{1}{N_a} \times R_a \times \left(\frac{N}{R_a}\right)^2 = 1 \rightarrow N_a = \frac{N^2}{R_a}$$

Pseudocode; basis construction

```
do s = 0, 2^N - 1
    call checkstate(s, R)
    if R ≥ 0 then a = a + 1; s_a = s; R_a = R endif
enddo
M = a
```

M = size of the H-block

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} e^{-ikr} T^r |a\rangle$$

Normalization of a state |*a*(k)> with periodicity R_a

$$\langle a(k)|a(k)\rangle = \frac{1}{N_a} \times R_a \times \left(\frac{N}{R_a}\right)^2 = 1 \rightarrow N_a = \frac{N^2}{R_a}$$

Pseudocode; basis construction

$$\begin{aligned}
&\textbf{do } s = 0, 2^N - 1 \\
&\quad \textbf{call checkstate}(s, R) \\
&\quad \textbf{if } R \geq 0 \textbf{ then } a = a + 1;\ s_a = s;\ R_a = R \textbf{ endif} \\
&\textbf{enddo} \\
&M = a
\end{aligned}$$

M = size of the H-block

Uses a subroutine **checkstate**(s,R)

- *R* = periodicity if state-integer s is a new representative
- store in list ***R***
- *R* = –1 if
  - the magnetization is not the one currently considered
  - some translation of |s> gives a state-integer smaller than s

Translations of the representative; cyclic permutation

Define function **cyclebits**(t,N)

- cyclic permutations of first N bits of integer t
- F90 function ishiftc(t,–1,N)

The representative has the lowest state-integer among all its translations

Pseudocode; checkstate() subroutine

subroutine checkstate(s, R)
$R = -1$
if $(\sum_i s[i] \neq n_\uparrow)$ **return** — check the magnetization
$t = s$
do $i = 1, N$
    $t =$ **cyclebits**(t, N) — check if translated state has lower integer representation
    if $(t < s)$ **then**
        return
    elseif $(t = s)$ **then**
        if $(\mathbf{mod}(k, N/i) \neq 0)$ **return** — check momentum compatibility
        $R = i$; **return**
    endif

- k is the integer corresponding to the momentum; k=0,...,N-1

The Hamiltonian matrix. Write $S = 1/2$ chain hamiltonian as

$$H_0 = \sum_{j=1}^{N} S^z_j S^z_{j+1}, \quad H_j = \tfrac{1}{2}(S^+_j S^-_{j+1} + S^+_j S^-_{j+1}), \ \ j = 1, \ldots, N$$

Act with H on a momentum state; use [H,T]=0

$$H|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r H|a\rangle = \frac{1}{\sqrt{N_a}} \sum_{j=0}^{N} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r H_j |a\rangle,$$

$H_j|a\rangle$ is related to some representative: $H_j|a\rangle = h^j_a T^{-l_j} |b_j\rangle$

$$H|a(k)\rangle = \sum_{j=0}^{N} \frac{h^j_a}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^{(r-l_j)} |b_j\rangle$$

Pseudocode; hamiltonian construction

First, some elements needed; recall

$$H_j|a\rangle = h_a^j T^{-l_j}|b_j\rangle$$

Finding the representative r of a state-integer s

- lowest integer among all translations

$$|r\rangle = T^l|s\rangle$$

subroutine representative(s, r, l)
$r = s;\ t = s;\ l = 0$
do $i = 1, N-1$
  $t =$ **cyclebits**(t, N)
  if $(t < r)$ **then** $r = t;\ l = i$ **endif**

subroutine findstate(s, b)
$b_{\min} = 1;\ b_{\max} = M$
do

$s =$ **flip**(s_a, i, j)
call representative(s, r, l)
call findstate(r, b)
if $(b \geq 0)$ **then**
  $H(a,b) = H(a,b) + \frac{1}{2}\sqrt{R_a/R_b}\mathrm{e}^{i2\pi kl/N}$
endif
endif
enddo
enddo

Construct all the matrix elements

```
do a = 1, M
    do i = 0, N − 1
        j = mod(i + 1, N)
        if (s_a[i] = s_a[j]) then
            H(a, a) = H(a, a) + 1/4
        else
            H(a, a) = H(a, a) − 1/4
            s = flip(s_a, i, j)
            call representative(s, r, l)
            call findstate(r, b)
            if (b ≥ 0) then
                H(a, b) = H(a, b) + 1/2 sqrt(R_a/R_b) e^{i2πkl/N}
            endif
        endif
    enddo
enddo
```

$$H(a,b) = H(a,b) + \frac{1}{2}\sqrt{R_a/R_b}\,\mathrm{e}^{i2\pi kl/N}$$

Reflection symmetry (parity) Define a reflection (parity) operator

$$P|S_1^z, S_2^z, \ldots, S_N^z\rangle = |S_N^z, \ldots, S_2^z, S_1^z\rangle$$

Consider a hamiltonian for which [H,P]=0 and [H,T]=0; but note that [P,T]≠0

Reflection symmetry (parity)

Define a reflection (parity) operator

$$P|S_1^z, S_2^z, \ldots, S_N^z\rangle = |S_N^z, \ldots, S_2^z, S_1^z\rangle$$

Consider a hamiltonian for which [H,P]=0 and [H,T]=0; but note that [P,T]≠0

Can we still exploit both P and T at the same time? Consider the state

$$|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r (1 + pP)|a\rangle, \quad p = \pm 1$$

Reflection symmetry (parity) Define a reflection (parity) operator

$$P|S_1^z, S_2^z, \ldots, S_N^z\rangle = |S_N^z, \ldots, S_2^z, S_1^z\rangle$$

Consider a hamiltonian for which [H,P]=0 and [H,T]=0; but note that [P,T]≠0

Can we still exploit both P and T at the same time? Consider the state

$$|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r (1 + pP)|a\rangle, \quad p = \pm 1$$

This state has momentum k, but does it have parity p? Act with P

$$P|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^{-r} (P + p)|a\rangle$$

$$= p\frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{ikr} T^r (1 + pP)|a\rangle \;\; = p|a(k,p)\rangle \text{ if } k = 0 \text{ or } k = \pi$$

Reflection symmetry (parity) Define a reflection (parity) operator

$$P|S_1^z, S_2^z, \ldots, S_N^z\rangle = |S_N^z, \ldots, S_2^z, S_1^z\rangle$$

Consider a hamiltonian for which [H,P]=0 and [H,T]=0; but note that [P,T]≠0

Can we still exploit both P and T at the same time? Consider the state

$$|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r (1+pP)|a\rangle, \quad p = \pm 1$$

This state has momentum k, but does it have parity p? Act with P

$$P|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^{-r} (P+p)|a\rangle$$

$$= p\frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{ikr} T^r (1+pP)|a\rangle \quad = p|a(k,p)\rangle \text{ if } k=0 \text{ or } k=\pi$$

k=0,π momentum blocks are split into p=+1 and p=–1 sub-blocks

- [T,P]=0 in the k=0,π blocks
- physically clear because -k=k on the lattice for k=0,π

Reflection symmetry (parity) Define a reflection (parity) operator

$$P|S_1^z, S_2^z, \ldots, S_N^z\rangle = |S_N^z, \ldots, S_2^z, S_1^z\rangle$$

Consider a hamiltonian for which [H,P]=0 and [H,T]=0; but note that [P,T]≠0

Can we still exploit both P and T at the same time? Consider the state

$$|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r (1+pP)|a\rangle, \quad p = \pm 1$$

This state has momentum k, but does it have parity p? Act with P

$$P|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^{-r} (P+p)|a\rangle$$

$$= p\frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{ikr} T^r (1+pP)|a\rangle \;\; = p|a(k,p)\rangle \text{ if } k=0 \text{ or } k=\pi$$

Reflection symmetry (parity) Define a reflection (parity) operator

$$P|S_1^z, S_2^z, \ldots, S_N^z\rangle = |S_N^z, \ldots, S_2^z, S_1^z\rangle$$

Consider a hamiltonian for which [H,P]=0 and [H,T]=0; but note that [P,T]≠0

Can we still exploit both P and T at the same time? Consider the state

$$|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r (1 + pP)|a\rangle, \quad p = \pm 1$$

This state has momentum k, but does it have parity p? Act with P

$$P|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^{-r} (P + p)|a\rangle$$

$$= p\frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{ikr} T^r (1 + pP)|a\rangle \quad = p|a(k,p)\rangle \text{ if } k = 0 \text{ or } k = \pi$$

k=0,π momentum blocks are split into p=+1 and p=–1 sub-blocks

- [T,P]=0 in the k=0,π blocks
- physically clear because -k=k on the lattice for k=0,π

Reflection symmetry (parity)

Define a reflection (parity) operator

$$P|S_1^z, S_2^z, \ldots, S_N^z\rangle = |S_N^z, \ldots, S_2^z, S_1^z\rangle$$

Consider a hamiltonian for which [H,P]=0 and [H,T]=0; but note that [P,T]≠0

Can we still exploit both P and T at the same time? Consider the state

$$|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r (1 + pP)|a\rangle, \quad p = \pm 1$$

This state has momentum k, but does it have parity p? Act with P

$$P|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^{-r} (P + p)|a\rangle$$

$$= p\frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{ikr} T^r (1 + pP)|a\rangle \;= p|a(k,p)\rangle \text{ if } k = 0 \text{ or } k = \pi$$

k=0,π momentum blocks are split into p=+1 and p=–1 sub-blocks

- [T,P]=0 in the k=0,π blocks
- physically clear because -k=k on the lattice for k=0,π

Semi-momentum states

Mix momenta +k and –k for k≠0,π. Introduce function

$$C_k^\sigma(r) = \begin{cases} \cos(kr), & \sigma = +1 \\ \sin(kr), & \sigma = -1. \end{cases}$$

Useful trigonometric relationships

$$\begin{aligned} C_k^\pm(-r) &= \pm C_k^\pm(r), \\ C_k^\pm(r+d) &= C_k^\pm(r)C_k^+(d) \mp C_k^\mp(r)C_k^-(d). \end{aligned}$$

Reflection symmetry (parity) Define a reflection (parity) operator

$$P|S_1^z, S_2^z, \ldots, S_N^z\rangle = |S_N^z, \ldots, S_2^z, S_1^z\rangle$$

Consider a hamiltonian for which [H,P]=0 and [H,T]=0; but note that [P,T]≠0

Reflection symmetry (parity) Define a reflection (parity) operator

$$P|S_1^z, S_2^z, \dots, S_N^z\rangle = |S_N^z, \dots, S_2^z, S_1^z\rangle$$

Consider a hamiltonian for which [H,P]=0 and [H,T]=0; but note that [P,T]≠0

Reflection symmetry (parity) Define a reflection (parity) operator

$$P|S_1^z, S_2^z, \ldots, S_N^z\rangle = |S_N^z, \ldots, S_2^z, S_1^z\rangle$$

Consider a hamiltonian for which [H,P]=0 and [H,T]=0; but note that [P,T]≠0

Can we still exploit both P and T at the same time? Consider the state

$$|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r (1 + pP)|a\rangle, \quad p = \pm 1$$

Reflection symmetry (parity)

Define a reflection (parity) operator

$$P|S^z_1, S^z_2, \ldots, S^z_N\rangle = |S^z_N, \ldots, S^z_2, S^z_1\rangle$$

Consider a hamiltonian for which [H,P]=0 and [H,T]=0; but note that [P,T]≠0

Can we still exploit both P and T at the same time? Consider the state

$$|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r (1 + pP)|a\rangle, \quad p = \pm 1$$

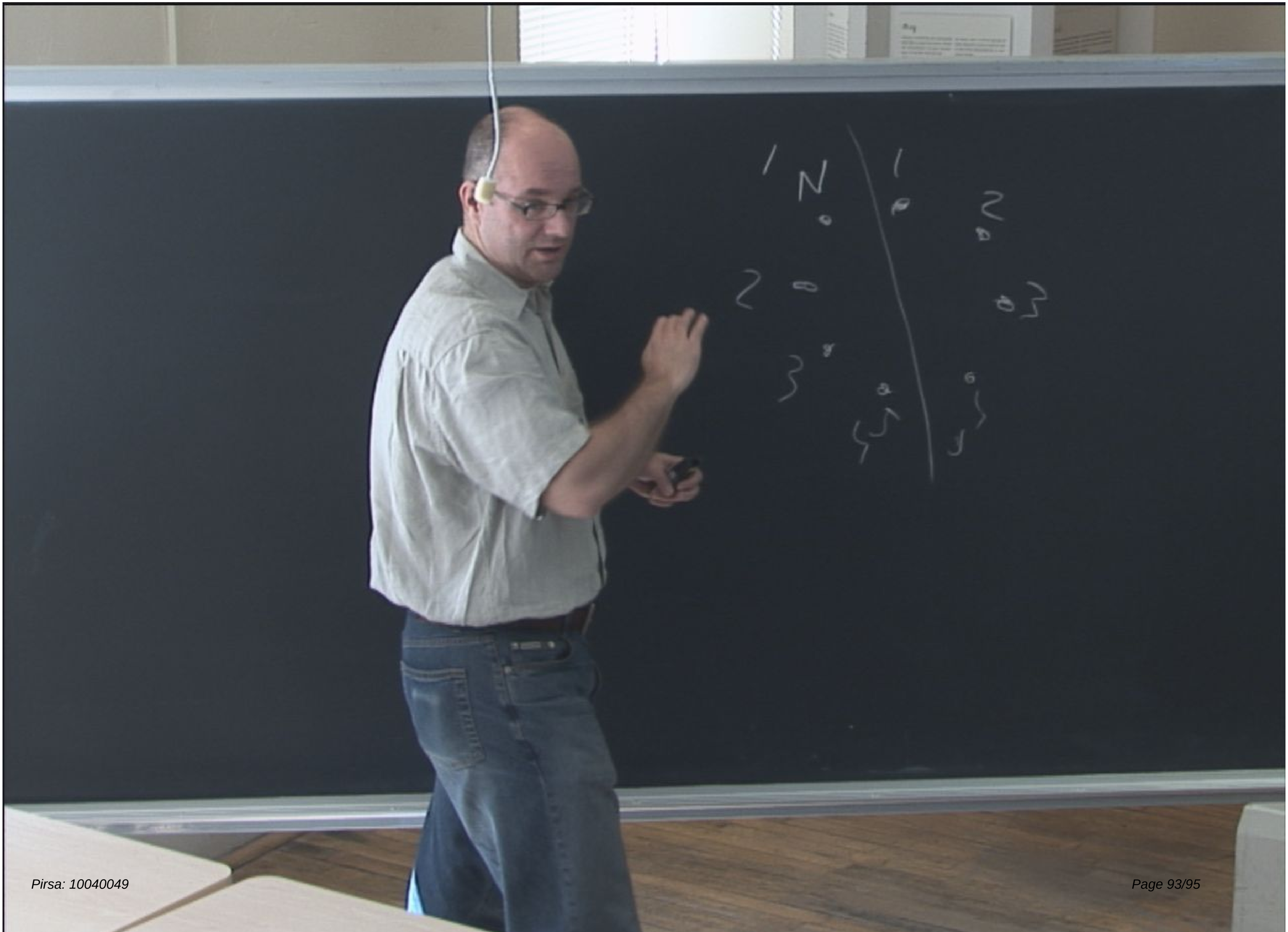
This state has momentum k, but does it have parity p? Act with P

$$P|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^{-r} (P + p)|a\rangle$$

$$= p \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{ikr} T^r (1 + pP)|a\rangle \; = p|a(k,p)\rangle \text{ if } k = 0 \text{ or } k = \pi$$

k=0,π momentum blocks are split into p=+1 and p=–1 sub-blocks

- [T,P]=0 in the k=0,π blocks
- physically clear because -k=k on the lattice for k=0,π



Reflection symmetry (parity)

Define a reflection (parity) operator

$$P|S_1^z, S_2^z, \ldots, S_N^z\rangle = |S_N^z, \ldots, S_2^z, S_1^z\rangle$$

Consider a hamiltonian for which [H,P]=0 and [H,T]=0; but note that [P,T]≠0

Can we still exploit both P and T at the same time? Consider the state

$$|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r (1+pP)|a\rangle, \quad p = \pm 1$$

This state has momentum k, but does it have parity p? Act with P

$$P|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^{-r} (P+p)|a\rangle$$

$$= p\frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{ikr} T^r (1+pP)|a\rangle \;= p|a(k,p)\rangle \text{ if } k = 0 \text{ or } k = \pi$$

k=0,π momentum blocks are split into p=+1 and p=–1 sub-blocks

- [T,P]=0 in the k=0,π blocks
- physically clear because -k=k on the lattice for k=0,π